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L4: Entry 1 of 1 File: DWPI Nov 5, 1996

DERWENT-ACC-NO: 1997-029480
DERWENT-WEEK: 200024

TITLE: Prepn. of optically active 2-propyl octanoic acid useful in treatment of neuro denaturation disease - comprises optical resolution of salts of racemic octanoic acid and amine, acid addn. and redn. to give higher yield(s)

PATENT-ASSIGNEE:

ASSIGNEE	CODE
ONO PHARM CO LTD	ONOY

PRIORITY-DATA: 1995JP-0098328 (April 24, 1995)

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PATENT-FAMILY:

PUB-NO	PUB-DATE	LANGUAGE	PAGES	MAIN-IPC
JP 08291106 A	November 5, 1996		006	C07C057/18
JP 3032447 B2	April 17, 2000		006	C07C057/18

APPLICATION-DATA:

PUB-NO	APPL-DATE	APPL-NO	DESCRIPTOR
JP 08291106A	April 24, 1995	1995JP-0098328	
JP 3032447B2	April 24, 1995	1995JP-0098328	
JP 3032447B2		JP 8291106	Previous Publ.

INT-CL (IPC): B01J 23/40; C07B 57/00; C07C 51/43; C07C 57/18; C07M 7/00

ABSTRACTED-PUB-NO: JP 08291106A
BASIC-ABSTRACT:

Prepn. of optically active 2-propyl octanoic acid comprises: (i) optical resolution of salts of racemic 2-(2-propynyl)octanoic acid and optically active amine; (ii) acid treatment of the obtd. salts; and (iii) redn. of the obtd. optically active 2-(2-propynyl) octanoic acid.

Reduction is pref. catalytic reduction. Optical resolution is pref. separation recrystallisation method.

USE/ADVANTAGE - Optically active 2-propyl octanoic acid is useful cpd. for medicine, effective for the prevention and treatment of neuro denaturation disease caused by abnormal function of astrocyte. The method gives the cpd. in three times

higher yield and higher purity with less number of recrystallisation than the conventional method.

Examples of optically active amine, starting materials, are (R)-(+)-1-phenethylamine, (R)-(+)-1-(4-methylphenyl)ethylamine, L-arginine, 2R-aminobutanol, (S)-(-)-nicotine, hydroquinine, dehydro-abiethylamine, etc. Optical resolution is carried out by separation recrystallisation or liquid column chromatography, etc. Reduction is carried out in an inert organic solvent under H2 atmosphere using catalyst such as palladium carbon, Pd, Pt, platinum oxide and Ni at 0-60 deg. C.

In an example, to (2RS)-2-(2-propynyl)octanoic acid (2.32 g, 12.7 mM) was added (R)-(+)-1-phenylethylamine (1.22 g), and the mixt. was dissolved in n-hexane (8 ml). The obtd. soln. was cooled slowly to give 2.33 g of crystals, which were further recrystallised 4 times using n-hexane to give 0.48 g of crystals. 1N HCl was added to thus obtd. crystals (267 mg), and the mixt. was extracted with n-hexane. The organic layer was treated by the ordinary method to give 160 mg of (2S)-2-(2-propynyl)octan- oic acid as colourless oily substance. 114 mg of the above obtained cpd. was dissolved in ethyl acetate (2 ml), and the whole was subjected to catalytic reduction using palladium carbon (10 mg) under H2 atmosphere at room temp. for 10 min. to give 113 mg of (2R)-2-propyl-octanoic acid. Optical purity: 90.0% e.e.

CHOSEN-DRAWING: Dwg.0/0

TITLE-TERMS: PREPARATION OPTICAL ACTIVE PROPYL OCTANOIC ACID USEFUL TREAT NEURO DENATURE DISEASE COMPRISE OPTICAL RESOLUTION SALT RACEMIC OCTANOIC ACID AMINE ACID ADD REDUCE HIGH YIELD

DERWENT-CLASS: B05

CPI-CODES: B10-C04E; B14-J01;

CHEMICAL-CODES:

Chemical Indexing M2 *01*
Fragmentation Code
A546 C810 M411 M730 M903 Q421 Q509

Chemical Indexing M2 *02*
Fragmentation Code
J0 J011 J1 J171 M220 M224 M232 M262 M281 M320
M416 M620 M720 M800 M903 M904 N214 N311 N412 N441
N480 N512 P446 P625
Markush Compounds
199703-17701-P

SECONDARY-ACC-NO:
CPI Secondary Accession Numbers: C1997-009151

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JP8291106

Publication Title:

PRODUCTION OF OPTICALLY ACTIVE 2-PROPYLOCTANOIC ACID

Abstract:

Abstract of JP8291106

PURPOSE: To provide a method for producing optically active 2-propyloctanoic acid in both higher chemical yield and optical purity than a method for separating the optical active substance from the racemic modification of the objective compound. CONSTITUTION: A salt prepared by using (2RS)-2-(2-propenyl)octanoic acid as a racemic modification and an optically active amine is subjected to optical resolution by fractional crystallization method. The prepared crystal is treated with an acid to give optically active (2R)-2-(2-propenyl)octanoic acid, which is reduced to give optically active (2R)-2-propyloctanoic acid. Data supplied from the esp@cenet database - Worldwide

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